# Application of Parallel Computing for Two- and Three-Dimensional Modeling of Bulk Crystal Growth and Microstructure Formation

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## Introduction

The quality of metal oxide and semiconductor crystals grown from the melt depends fundamentally on heat, mass, and species transport in the melt and crystal and on the interactions of these fields with the formation of microstructure, microdefects, dislocations, and voids in the grown crystal. Modeling of these individual processes for understanding their complex interactions is essential to the successful growth of crystals in a microgravity environment and to the interpretation of experiments from ground-based and microgravity research. The complexity of mathematical models of these phenomena makes numerical simulation essential. The goal of this project is to develop modern numerical simulation methods for calculation of complex models of transport processes in crystal growth and of microdefect formation using modern scaleable parallel computing.

Research to date has focused on the development of numerical methods for two types of mathematical models: development of parallel numerical algorithms for solutions of complex models of transport processes in material processing, and the development of algorithms for computation of mesoscale microstructure in materials processing. In parallel, we have continued our investigation of the dynamics of small-scale crystal growth systems of interest in microgravity applications, especially of the thermal-capillary and hydrodynamic dynamics of small-scale floating zone systems. This later research will not be discussed in this report.

## Parallel Solution of Materials Processing Models

In the first study, implementation of scaleable parallel numerical algorithms are developed for the solution of the large, sparse systems of linear algebraic equations that arise when Newton's method is applied to the solution of the nonlinear algebraic equations formed from finite element discretization of transport problems, such as the description of natural convection in crystal growth melts, or of the free-boundary problem that describes heat transfer, phase change, and convection in solidification systems. Here we have focused on the development of Schwarz-Krylov methods for solution of the discrete modified-Stokes problems that arise at Newton iterations of nonlinear fluid mechanical problems. We have developed a block preconditioned Krylov iterative method based on the bi-conjugate gradient stabilized (Bi-CGSTAB) algorithm. The preconditioner is a Schur compliment factorization of the Jacobian based on the pressure variables and coupled with an additive Schwarz, domain decomposition iterative solution of the associated linear system. A coarse-grid preconditioner for the pressure variables also is used and direct LU decomposition is applied to the coarse-grid problem and to the domain-sized problems within the additive Schwarz method. This block-preconditioned Bi-CGSTAB method was implemented for a prototype problem of nonlinear, two-dimensional natural convection and tested on a single processor Hewlett Packard 735 computer. The iterative method compared well with a state-of-the-art direct solution method for varying Grashof number. Because the i of Schwarz-Krylov method does not require the storage of any zeros, larger problem sizes also are tractable than for the direct method.

The Schwarz-Krylov method was implemented in parallel using the recursive spectral dissection method to partition elements to processors, as implemented in the program CHACO. The code was written in the MPI language. Parallel efficiencies scaled well with increasing problem size and number of processors. These results suggest that the Schwarz-Krylov method will be robust for the solution of much more complex materials processing problems; application to a representative solidification problem is underway.

Parallel Simulation of Microstructure in Silicon Crystals

The second class of applications has been the development of models and numerical algorithms for simulation of microdefect formation in crystalline silicon, as occurs during the cooling during Czochralski and floating zone crystal growth. Although commercial semiconductor silicon is nearly perfect, comparison of the predictions of our models with experiments have shown that native point defects — self-interstitials and vacancies — in silicon diffuse, combine, and aggregate to form mesoscopic clusters that affect semiconductor device performance. We have constructed models of point defect dynamics and aggregation using statistical mechanical concepts for diffusion-limited reaction to model the interactions of point defects as chemical reactions. The distribution of point defect aggregates is modeled by combining discrete kinetic rate equations for small cluster sizes ($n < 20$) and a continuous size distribution governed by a Fokker-Planck equation for the description of very large cluster sizes ($20 < n < 1 \times 10^{10}$). The numerical solution of these equations combines two very different discretizations: a variable finite difference approximation constructed to maintain the monotonicity of the continuous cluster size distribution for discretization of the $n$-space Fokker-Planck equation and a Galerkin finite element discretization of variables in physical space. Because clusters of point defects cannot diffuse, the Fokker-Planck and discrete rate equations describing their dynamical evolution are hyperbolic equations in physical space and diffusive only in the state-space $n$ of the size distribution, as written in the Fokker-Planck equation.

The solution of these models involves parallel implementation transient methods for simultaneous solution of the models describing point defect formation and aggregation. We have developed a mesoscale-macroscale splitting method for time integration formed from a couple discontinuous finite element/finite-volume solution of the Fokker-Planck equation and discrete rate equations for the non-diffusing clusters with an implicit transient finite element analysis of the reaction-diffusion point defect equations. The result gives a decoupled algorithm in which the discretized representations of the defect distributions are easily computed sequentially at each point in the crystal, and so are very amenable to parallel computing by considering simultaneous solution along parallel solution characteristics. This approach, coupled with implementation of the Schwarz-Krylov method for solution of the discrete-diffusion reaction problem, will yield a highly parallel and robust algorithm for simulating very complex microdefect formulation.

The application of these models is already bearing fruit. Comparison of experiments and quasi-one-dimensional simulations for the formation of microvoids — voids in silicon of 50 to 500 nm in radius — that are formed by vacancy aggregation during crystal growth show the accuracy of the calculations for predicting the formation of these defects in silicon and for connecting microdefect formation with macroscale processing conditions. These simulations are the first detailed description of the formation of microdefects in silicon and are the foundation for detailed analysis of the evolution of defects throughout silicon processing. The parallel transient analysis will yield the first fully two-dimensional simulation of microdefect dynamics in silicon.